Mauro Ferrario

List of Publications by Year
in descending order

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121 papers	4,326 citations	126907 33 h-index	114465 63 g-index
128 all docs	128 docs citations	128 times ranked	3086 citing authors

#	Article	IF	Citations
1	Molecular-dynamics simulation of liquid methanol. The Journal of Physical Chemistry, 1987, 91, 4934-4940.	2.9	420
2	Molecularâ€dynamics simulation of aqueous mixtures: Methanol, acetone, and ammonia. Journal of Chemical Physics, 1990, 93, 5156-5166.	3.0	378
3	Molecular dynamics of rigid systems in cartesian coordinates A general formulation. Molecular Physics, 1982, 47, 1253-1264.	1.7	318
4	Constrained molecular dynamics and the mean potential for an ion pair in a polar solvent. Chemical Physics, 1989, 129, 241-251.	1.9	234
5	Dynamics of ion pair interconversion in a polar solvent. Journal of Chemical Physics, 1990, 93, 7137-7147.	3.0	179
6	Molecular dynamics study of a sodium octanoate micelle in aqueous solution. The Journal of Physical Chemistry, 1988, 92, 819-821.	2.9	151
7	Molecular dynamics simulation of electron-transfer reactions in solution. The Journal of Physical Chemistry, 1989, 93, 6261-6265.	2.9	138
8	Constant pressure-constant temperature molecular dynamics for rigid and partially rigid molecular systems. Molecular Physics, 1985, 54, 587-603.	1.7	125
9	Molecularâ€dynamics study of adiabatic protonâ€transfer reactions in solution. Journal of Chemical Physics, 1992, 97, 378-388.	3.0	111
10	Constant pressure-constant temperature molecular dynamics: a correct constrained NPT ensemble using the molecular virial. Molecular Physics, 2003, 101, 765-778.	1.7	103
11	Ab initiostudy on the surface chemistry and nanotribological properties of passivated diamond surfaces. Physical Review B, 2009, 79, .	3.2	91
12	Solubility of KF in water by molecular dynamics using the Kirkwood integration method. Journal of Chemical Physics, 2002, 117, 4947-4953.	3.0	87
13	The structure of liquid benzene. Molecular Physics, 1983, 50, 217-227.	1.7	82
14	Pair interactions and hydrogen-bond networks in models of liquid methanol. Molecular Physics, 1986, 58, 849-853.	1.7	77
15	Blue Moon Approach to Rare Events. Molecular Simulation, 2004, 30, 787-793.	2.0	69
16	The nonâ€Markovian relaxation process as a â€˜â€˜contractionâ€™â€™ of a multidimensional one of Markovian type. Journal of Mathematical Physics, 1979, 20, 2567-2572.	1.1	67
17	Activation energies by molecular dynamics with constraints. Chemical Physics Letters, 1991, 176, 581-587.	2.6	67
18	Density Functional Study of the Photoactive Yellow Protein's Chromophore. Journal of Physical Chemistry B, 2001, 105, 4386-4391.	2.6	59

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19	Diffusion effects of hydrogen bond fluctuations. I. The long time regime of the translational and rotational diffusion of water. Journal of Chemical Physics, 1989, 91, 1179-1190.	3.0	55
20	Non-Hamiltonian equations of motion with a conserved energy. Physical Review E, 2001, 64, 056125.	2.1	53
21	Dynamical behavior of the azide ion in protic solvents. Chemical Physics Letters, 1993, 213, 537-540.	2.6	50
22	Anion ordering in alkali cyanide crystals. Journal of Chemical Physics, 1986, 84, 3975-3985.	3.0	42
23	Dynamical Properties of Hydrogen-Bonded Liquids. Advances in Chemical Physics, 2007, , 277-320.	0.3	42
24	Dynamical Non-Equilibrium Molecular Dynamics. Entropy, 2014, 16, 233-257.	2.2	41
25	A molecular dynamics study of orientational disordering in crystalline sodium nitrate. Journal of Physics Condensed Matter, 1989, 1, 6523-6542.	1.8	40
26	Spectroscopic and molecular dynamics studies of solvation of cyanomethane and cyanide ions. Faraday Discussions of the Chemical Society, 1988, 85, 237-253.	2.2	39
27	Shear-rate dependence of the viscosity of the Lennard-Jones liquid at the triple point. Physical Review A, 1991, 44, 6936-6939.	2.5	39
28	Structure of NaCl and KCl concentrated aqueous solutions byab initiomolecular dynamics. Molecular Physics, 2004, 102, 959-966.	1.7	38
29	Monitoring water and oxygen splitting at graphene edges and folds: Insights into the lubricity of graphitic materials. Carbon, 2020, 156, 93-103.	10.3	38
30	Simulation of site-site soft-core liquid crystal models. Molecular Physics, 1993, 80, 297-312.	1.7	37
31	Pressure Induced Friction Collapse of Rare Gas Boundary Layers Sliding over Metal Surfaces. Physical Review Letters, 2007, 99, 176101.	7.8	37
32	A molecular dynamics study of the TIP4P model of water. Chemical Physics Letters, 1985, 121, 182-186.	2.6	35
33	Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties. Chemical Physics, 1982, 72, 141-145.	1.9	34
34	Activation free energy for proton transfer in solution. Chemical Physics, 1994, 180, 181-189.	1.9	34
35	Onset of frictional slip by domain nucleation in adsorbed monolayers. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1311-1316.	7.1	32
36	Statistical geometry of hard particles on a sphere. Physica A: Statistical Mechanics and Its Applications, 1992, 187, 456-474.	2.6	31

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37	Statistical geometry of hard particles on a sphere: analysis of defects at high density. Physica A: Statistical Mechanics and Its Applications, 1993, 201, 649-665.	2.6	30
38	Rare events by constrained molecular dynamics. Journal of Molecular Liquids, 2000, 89, 1-18.	4.9	30
39	Non-equilibrium by molecular dynamics: a dynamical approach. Molecular Simulation, 2016, 42, 1385-1400.	2.0	30
40	A generalization of the kuboâ€"freed relaxation theory. Chemical Physics Letters, 1979, 62, 100-106.	2.6	29
41	Simulation of superoxide-superoxide dismutase association rate for six natural variants. Comparison with the experimental catalytic rate. The Journal of Physical Chemistry, 1994, 98, 10554-10557.	2.9	28
42	Solvent-solute hydrogen bonding in dilute solutions of CN-and CH3CN in water and methanol. Molecular Physics, 1992, 77, 617-627.	1.7	27
43	Effective binding force calculation in a dimeric protein by molecular dynamics simulation. Journal of Chemical Physics, 2002, 116, 6329-6338.	3.0	27
44	Dynamics-Function Correlation in Cu, Zn Superoxide Dismutase: A Spectroscopic and Molecular Dynamics Simulation Study. Biophysical Journal, 2001, 80, 2556-2567.	0.5	26
45	Cation transport in lithium sulphate based crystals. Molecular Physics, 1995, 86, 923-938.	1.7	25
46	Computer simulation of dichloromethane. II. Molecular dynamics. Chemical Physics, 1982, 72, 147-154.	1.9	24
47	A Microscopic Description of Concentrated Potassium Fluoride Aqueous Solutions by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2003, 107, 2354-2361.	2.6	24
48	Computer simulation of the generalized brownian motion. Molecular Physics, 1982, 46, 875-889.	1.7	23
49	Ideal adhesive and shear strengths of solid interfaces: A high throughput ab initio approach. Computational Materials Science, 2018, 154, 517-529.	3.0	22
50	The mutual interaction of molecular rotation and translation. Molecular Physics, 1980, 39, 1369-1389.	1.7	19
51	Hydrogen bond statistics and dynamics in water: Selfâ€diffusion and dielectric relaxation. Journal of Chemical Physics, 1984, 81, 6214-6223.	3.0	19
52	Structural fluctuations and the order-disorder phase transition in calcite. Journal of Physics Condensed Matter, 1994, 6, 1345-1358.	1.8	19
53	Structural Transition on Cooling of Plastic Adamantane: A Molecular-Dynamics Study. Physical Review Letters, 1987, 59, 2574-2577.	7.8	18
54	Static and dynamic water molecules in Cu,Zn superoxide dismutase. Proteins: Structure, Function and Bioinformatics, 2003, 51, 607-615.	2.6	18

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55	Potential energy surface for rare gases adsorbed on Cu(111): parameterization of the gas/metal interaction potential. Journal of Physics Condensed Matter, 2007, 19, 305008.	1.8	18
56	Lubricated friction on nanopatterned surfaces via molecular dynamics simulations. Physical Review B, 2008, 77, .	3.2	18
57	Reversible integrators for basic extended system molecular dynamics. Molecular Physics, 1999, 97, 825-832.	1.7	15
58	Thermal Diffusion in Binary Mixtures: Transient Behavior and Transport Coefficients from Equilibrium and Nonequilibrium Molecular Dynamics. Langmuir, 2017, 33, 11281-11290.	3.5	15
59	High-throughput screening of the static friction and ideal cleavage strength of solid interfaces. Scientific Reports, 2019, 9, 17062.	3.3	15
60	Long-time tails in two-dimensional fluids by molecular dynamics. Physica A: Statistical Mechanics and Its Applications, 1997, 240, 268-276.	2.6	12
61	On the configurational temperature NosÃ¨â€“Hoover thermostat. Physica A: Statistical Mechanics and Its Applications, 2016, 461, 19-35.	2.6	12
62	Effective Binding Force Calculation in Dimeric Proteins. Molecular Simulation, 2004, 30, 807-816.	2.0	11
63	Nonlinear mobility of a driven system: Temperature and disorder effects. Surface Science, 2007, 601, 3676-3681.	1.9	11
64	Brownian motion with superimposed interaction: cosine potential and molecular dynamics simulation. Advances in Molecular Relaxation and Interaction Processes, 1981, 20, 1-10.	0.5	10
65	Probability diffusion in non-Markhovian, non-Gaussian molecular ensembles: A theoretical analysis and computer simulation. Zeitschrift FÃ¼r Physik B Condensed Matter and Quanta, 1981, 41, 165-176.	1.9	10
66	Role of rotational thermal bath excitation on the EPR transient regime: A theoretical discussion. Journal of Chemical Physics, 1981, 74, 235-245.	3.0	9
67	A â€œmicroscopicâ€•model for the dynamics of water. Chemical Physics Letters, 1983, 98, 548-553.	2.6	9
68	Non-linear effects in rotational dynamics in the liquid state. Molecular Physics, 1984, 53, 1251-1272.	1.7	9
69	A molecular dynamics study of the rotator phase of t-butyl bromide. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 2097.	1.1	9
70	Nonlinear Effects in Molecular Dynamics of the Liquid State. Advances in Chemical Physics, 2007, , 225-275.	0.3	9
71	First-Principle Molecular Dynamics of Sliding Diamond Surfaces: Tribochemical Reactions with Water and Load Effects. Journal of Low Temperature Physics, 2016, 185, 174-182.	1.4	9
72	On the establishment of thermal diffusion in binary Lennard-Jones liquids. European Physical Journal: Special Topics, 2016, 225, 1629-1642.	2.6	9

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73	Holonomic Constraints: A Case for Statistical Mechanics of Non-Hamiltonian Systems. Computation, 2018, 6, 11.	2.0	9
74	Quantum Mechanics/Molecular Mechanics (QM/MM) applied to tribology: Real-time monitoring of tribochemical reactions of water at graphene edges. Computational Materials Science, 2020, 173, 109400.	3.0	9
75	Molecular dynamics simulation of liquid CH2Cl2 with 3Ã—3 and 5Ã—5 site-site interactions. Advances in Molecular Relaxation and Interaction Processes, 1982, 22, 245-249.	0.5	8
76	Computer simulation of the molecular dynamics of liquid dichloro methane. Advances in Molecular Relaxation and Interaction Processes, 1982, 24, 75-105.	0.5	8
77	Structure of solid tâ€butyl cyanide: A study by means of constantâ€temperature, constantâ€pressure, molecularâ€dynamics simulations. Journal of Chemical Physics, 1987, 87, 4823-4828.	3.0	8
78	Size-dependent commensurability and its possible role in determining the frictional behavior of adsorbed systems. Physical Chemistry Chemical Physics, 2016, 18, 28997-29004.	2.8	8
79	Reversible integrators for basic extended system molecular dynamics. Molecular Physics, 1999, 97, 825-832.	1.7	8
80	SIMULATION OF CLASSICAL AND QUANTUM ACTIVATED PROCESSES IN THE CONDENSED PHASE. , 1995, , 150-190.		8
81	Structure of solid tâ€butyl cyanide: Interpretation of experimental data by means of molecular dynamics simulation. Journal of Chemical Physics, 1985, 83, 4726-4733.	3.0	7
82	Molecular dynamics simulation of ion association reactions in a polar solvent. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1988, 85, 925-929.	0.2	7
83	Theory of transient response for arbitrarily strong driving fields. Journal of the Chemical Society, Faraday Transactions 2, 1980, 76, 542.	1.1	6
84	Molecular dynamics of CH2Cl2: temperature dependences of the far infra-red spectrum. Part 1: experimental and simulation. Advances in Molecular Relaxation and Interaction Processes, 1982, 22, 79-87.	0.5	6
85	Molecular dynamics study of the plastic-crystalline phase transition of tetraphosphorus triselenide. Molecular Physics, 1995, 84, 727-742.	1.7	6
86	Partially folded states of HIV-1 protease: Molecular dynamics simulations and ligand binding. Computational and Theoretical Chemistry, 2006, 769, 111-121.	1.5	6
87	Ab initio calculation of adhesion and potential corrugation of diamond (001) interfaces. Computer Physics Communications, 2011, 182, 1796-1799.	7.5	6
88	A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. Molecular Physics, 2021, 119, .	1.7	6
89	The intermolecular dimer potential of non-dipolar linear molecules. Advances in Molecular Relaxation and Interaction Processes, 1981, 20, 215-231.	0.5	5
90	Dielectric relaxation as a multiplicative stochastic process. Physica A: Statistical Mechanics and Its Applications, 1982, 111, 255-272.	2.6	5

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91	The correlation of molecular rotational and translational kinetic energy in liquid CH2Cl2 and CHCl3. Advances in Molecular Relaxation and Interaction Processes, 1982, 23, 69-73.	0.5	5
92	Correlation times for liquid CH2Cl2. Advances in Molecular Relaxation and Interaction Processes, 1982, 23, 113-117.	0.5	5
93	Orientational Disorder and Structural Phase Transitions in Plastic Molecular Crystals. , 1991, , 381-393.		5
94	Quantum effects on the solvent contribution to the activation free energy. Journal of Molecular Liquids, 1994, 61, 37-47.	4.9	5
95	Structure of phosphorus-selenium glasses: results fromab initiomolecular dynamics simulations. Molecular Physics, 2000, 98, 701-707.	1.7	5
96	Intermolecular pair and trimer potentials for methyl fluoride. Advances in Molecular Relaxation and Interaction Processes, 1981, 20, 47-62.	0.5	4
97	High-throughput generation of potential energy surfaces for solid interfaces. Computational Materials Science, 2022, 207, 111302.	3.0	4
98	Cumulant expansion of the orientational auto-correlation function. Advances in Molecular Relaxation and Interaction Processes, 1981, 19, 129-143.	0.5	3
99	Cybernetic spectroscopy of molecular rototranslation in the liquid state. Advances in Molecular Relaxation and Interaction Processes, 1982, 24, 139-148.	0.5	3
100	Non-Gaussian effects in the computer simulation of dichloro methane. Journal of Molecular Liquids, 1983, 26, 249-260.	4.9	3
101	First-principles simulation of phosphorus-selenium systems. Chemical Physics Letters, 1996, 259, 301-306.	2.6	3
102	Experimental and Simulative Dissociation of Dimeric Cu,Zn Superoxide Dismutase Doubly Mutated at the Intersubunit Surface. Biophysical Journal, 2005, 88, 2875-2882.	0.5	3
103	Coarse-graining stiff bonds. European Physical Journal: Special Topics, 2011, 200, 107-129.	2.6	3
104	Environmental Dynamics and Electron Transfer Reactions. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1990, , 133-148.	0.2	3
105	Non-gaussian distributions in computer triatomics. Chemical Physics Letters, 1980, 71, 139-144.	2.6	2
106	Numerical solution of fokker/planck/kramers equations. Advances in Molecular Relaxation and Interaction Processes, 1982, 23, 143-178.	0.5	2
107	Interaction of Cl2 molecules with GaAs(110) surface. Surface Science, 1998, 402-404, 47-51.	1.9	2
108	Introduction: Condensed Matter Theory by Computer Simulation. , 2006, , 1-11.		2

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109	Probabilistic Derivation of Spatiotemporal Correlation Functions in the Hydrodynamic Limit. Journal of Physical Chemistry B, 2016, 120, 1996-2000.	2.6	2
110	Molecular Dynamics vs. Stochastic Processes: Are We Heading Anywhere?. Entropy, 2018, 20, 348.	2.2	2
111	A theory of the dielectric loss in the aligned nematic mesophase. Physica A: Statistical Mechanics and Its Applications, 1981, 108, 135-142.	2.6	1
112	A spectrometer for far i.r. hot broad band fluorescence in gases. Spectrochimica Acta Part A: Molecular Spectroscopy, 1981, 37, 123-127.	0.1	1
113	Itinerant oscillation with a cosine potential. Chemical Physics, 1981, 62, 481-487.	1.9	1
114	Constrained and nonequilibrium molecular dynamics. , 1998, , .		1
115	Molecular dynamics simulations of the Trp repressorâ€“DNA complex and the AV77 mutant. Computer Physics Communications, 2005, 169, 130-134.	7.5	1
116	Scientific Visualization, a User View. , 1993, , 497-503.		0
117	Nonadiabatic molecular dynamics methods for diffusion. , 1998, , .		0
118	Condensed matter theory by computer simulation: from materials to chemical biology features. Europhysics News, 2007, 38, 18-22.	0.3	0
119	Boundary-lubricated friction in presence of a nano-well. Journal of Materials Science, 2008, 43, 3435-3440.	3.7	0
120	Correction for Reguzzoni et al., Onset of frictional slip by domain nucleation in adsorbed monolayers. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5693-5693.	7.1	0
121	Transient behavior of a model fluid under applied shear. Journal of Chemical Physics, 2013, 138, 184501.	3.0	0